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# Bis(1*H*-benzimidazole-$\kappa N^3$)bis[2-(naphthalen-1-yl)acetato-$\kappa^2 O,O'$]-nickel(II) monohydrate

**Fu-Jun Yin,[a]* Li-Jun Han,[b] Zhao Hong,[c] Xing-You Xu[d] and Li Ren[e]**

[a]Jiangsu Marine Resources Development Research Institute, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, [b]Department of Mathematics and Science, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, [c]Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, [d]Huaiyin Insititute of Technology, Huaiyin 223003, People's Republic of China, and [e]Qian'an College, Hebei United University, Tangshan 063009, People's Republic of China
Correspondence e-mail: yfj1999@126.com

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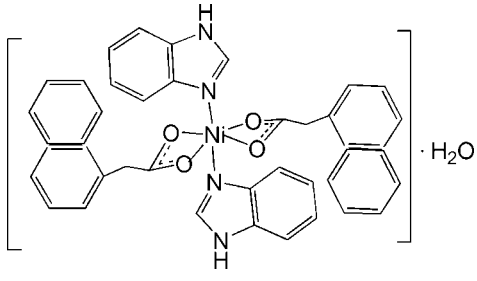
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.050; $wR$ factor = 0.122; data-to-parameter ratio = 12.7.

In the title compound, $[Ni(C_{12}H_9O_2)_2(C_7H_6N_2)_2]\cdot H_2O$, The $Ni^{II}$ cation is located on a twofold rotation axis and is six-coordinated in a distorted $NiN_2O_4$ octahedral geometry. The asymmetric unit consists of a nickel(II) ion, one 2-(naphthalen-1-yl)acetate anion, a neutral benzotriazole ligand and one half of a lattice water molecule. The crystal packing is stabilized by O—H···O and N—H···O hydrogen bonds. The title compound is isotypic with its $Cd^{II}$ analogue.

## Related literature

For the crystal structures of related 2-(naphthalen-1-yl)acetate complexes, see: Yin *et al.* (2011*a*,*b*); Liu *et al.* (2007); Yang *et al.* (2008); Tang *et al.* (2006); Ji *et al.* (2011). For the isotypic $Cd^{II}$ complex, see: Duan *et al.* (2007).



## Experimental

### Crystal data

$[Ni(C_{12}H_9O_2)_2(C_7H_6N_2)_2]\cdot H_2O$ $M_r$ = 683.37
Monoclinic, $C2/c$
$a$ = 11.573 (4) Å
$b$ = 19.991 (7) Å
$c$ = 14.290 (5) Å
$\beta$ = 105.903 (4)°
$V$ = 3179.5 (19) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.66 mm$^{-1}$
$T$ = 298 K
0.10 × 0.10 × 0.10 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.952, $T_{max}$ = 0.952
11840 measured reflections
2807 independent reflections
1849 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.083

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.122
$S$ = 0.99
2807 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.43 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$A$···O4 | 0.90 (8) | 2.24 (8) | 2.988 (6) | 141 (8) |
| N2—H2···O4$^{i}$ | 0.86 | 2.00 | 2.791 (4) | 152 |

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2448).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, m416 [doi:10.1107/S1600536812010021]

# Bis(1*H*-benzimidazole-$\kappa N^3$)bis[2-(naphthalen-1-yl)acetato-$\kappa^2 O,O'$]nickel(II) monohydrate

**Fu-Jun Yin, Li-Jun Han, Zhao Hong, Xing-You Xu and Li Ren**

## Comment

In recent years particular interest has been devoted to the 1-naphthylacetate ligand in coordination chemistry due to its ability to form metal complexes (Yin *et al.*, 2011*a*, 2011*b*; Liu *et al.*,2007; Yang *et al.*, 2008; Tang *et al.*,2006 ; Ji *et al.*, 2011). The crystal structure of the title compound was determined as part of an ongoing study of the properties of nickel complexes containing imidazole ligands. In the title mononuclear metal complex, the asymmetric unit consists of a nickel cation, one 2-(naphthalen-1-yl)acetate anion,a benzotriazole ligand, and half of a lattic water molecule. The $Ni^{II}$ cation is located on a two fold rotation axis and is six coordinated by two N from two benzotriazoles and four O atoms from two different 2-(naphthalen-1-yl)acetate anions, displaying a distorted NiN2O4 octahedral geometry, with Ni-O bond lengths in the range 2.056 (2)-2.288 (2)Å; the Ni-N bond length is 2.020 (3)Å. The crystal packing is stabilized by intermolecular N—H···O hydrogen bonding (Fig. 2) interactions which give rise to a one-dimensional chain structure. An isotypic cadmium(II) structure has been reported previously (Duan *et al.*, 2007).

## Experimental

The title compound was synthesized by the reaction of$Ni(NO_3)_2.6H_2O$, (87.24 mg, 0.3 mmol), 1-naphthylacetic acid(93 mg, 0.5 mmol), benzotriazole (35.4mg, 0.3 mmol) and NaOH (20 mg, 0.5 mmol) in 16 mL of a water-ethanol (2:1) mixture under solvothermal conditions. The mixture was homogenized and transferred into a sealed Teflon-lined solvothermal bomb (volume: 25 ml) and heated to 160°C for three days. After cooling colorless the crystals of the title compound were obtained, which were washed with distilled water and absolute ethanol.

## Refinement

H atoms were placed in calculated positions, with N–H = 0.86 Å ; C—H = 0.93 Å or C—H = 0.97 Å and refined with a riding model, with $U_{iso}$(H) = 1.2$U_{eq}$(C).Water H atoms were located in Fourier difference maps and refined isotropically..

## Computing details

Data collection: *APEX2* (Bruker 2008); cell refinement: *SAINT* (Bruker 2008); data reduction: *SAINT* (Bruker 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008.

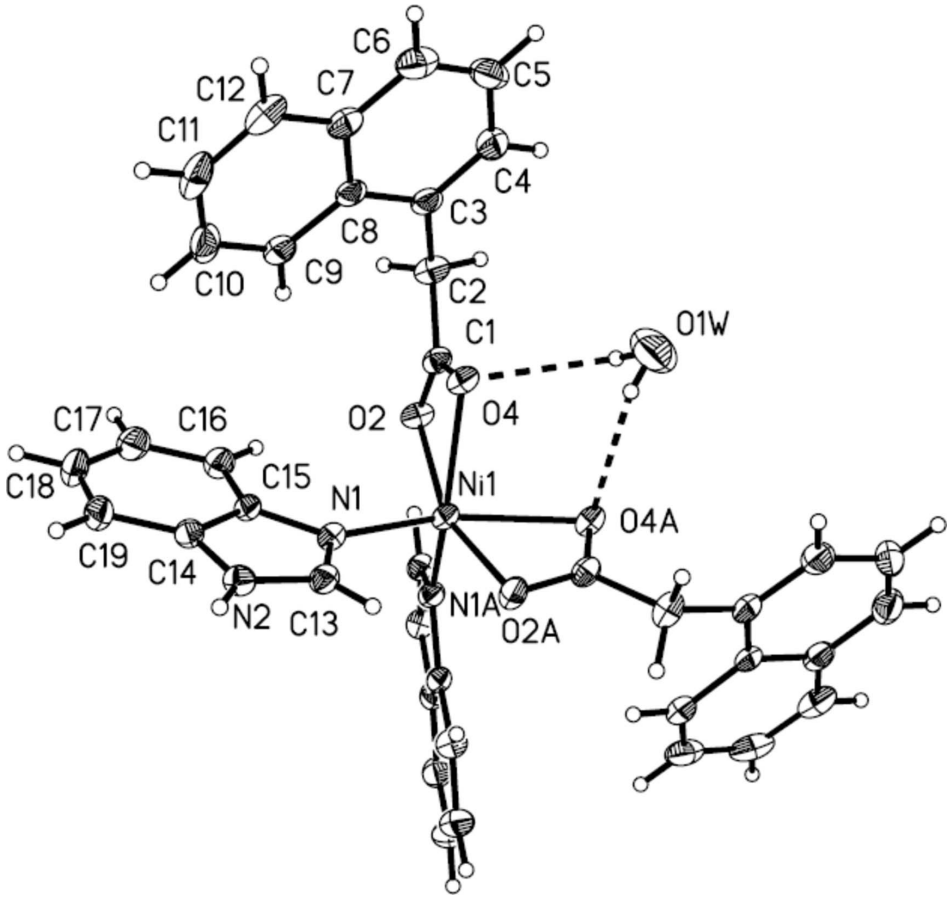


**Figure 1**

Molecule and the asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level.Hydrogenbonding is shown as dashed lines[Symmetry code: (A) 1-*x*, *y*, 1.5-*z*].

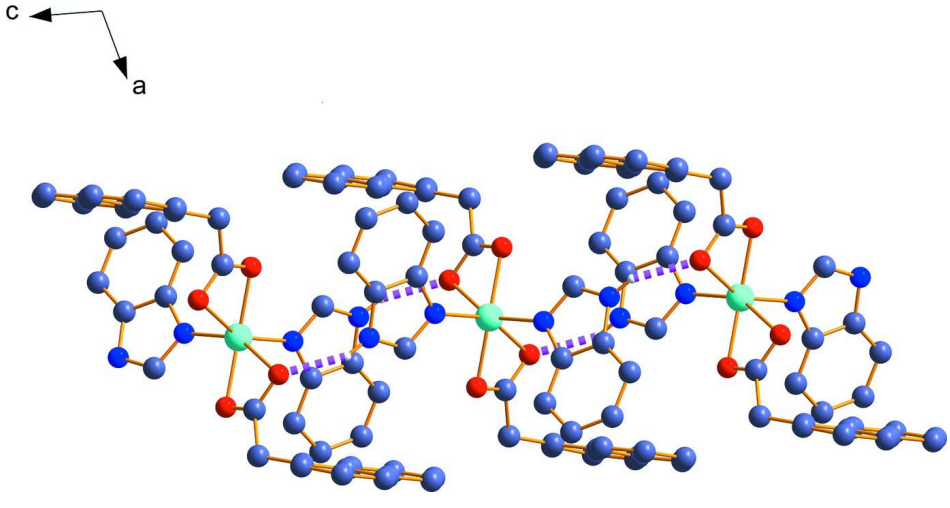


**Figure 2**

Part of the one-dimensional chain structure of (I) formed by N—H···O hydrogen bonds (dashed lines)along [001].

**Bis(1*H*-benzimidazole-$\kappa N^3$)bis[2-(naphthalen-1-yl)acetato-$\kappa^2 O,O'$]nickel(II) monohydrate**

*Crystal data*

$[Ni(C_{12}H_9O_2)_2(C_7H_6N_2)_2]\cdot H_2O$
$M_r = 683.37$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 11.573$ (4) Å
$b = 19.991$ (7) Å
$c = 14.290$ (5) Å
$\beta = 105.903$ (4)°
$V = 3179.5$ (19) Å$^3$
$Z = 4$
$F(000) = 1424$
$D_x = 1.428$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1368 reflections
$\theta = 3.5$–$23.4°$
$\mu = 0.66$ mm$^{-1}$
$T = 298$ K
Block, colourless
0.10 × 0.10 × 0.10 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.952$, $T_{max} = 0.952$
11840 measured reflections
2807 independent reflections
1849 reflections with $I > 2\sigma(I)$
$R_{int} = 0.083$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -13\rightarrow13$
$k = -23\rightarrow23$
$l = -16\rightarrow16$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.122$
$S = 0.99$
2807 reflections
221 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å$^{-3}$
$\Delta\rho_{min} = -0.43$ e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2$sigma($F^2$) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.6876 (3) | 0.58948 (19) | 0.7714 (2) | 0.0396 (9) |
| C2 | 0.8061 (3) | 0.6268 (2) | 0.7974 (3) | 0.0527 (10) |
| H2A | 0.8067 | 0.6572 | 0.8505 | 0.063* |
| H2B | 0.8701 | 0.5946 | 0.8214 | 0.063* |

| | | | | |
|---|---|---|---|---|
| C3 | 0.8350 (3) | 0.6664 (2) | 0.7174 (3) | 0.0460 (9) |
| C4 | 0.8408 (3) | 0.7344 (2) | 0.7213 (3) | 0.0585 (11) |
| H4 | 0.8252 | 0.7564 | 0.7738 | 0.070* |
| C5 | 0.8696 (4) | 0.7721 (2) | 0.6480 (4) | 0.0679 (13) |
| H5 | 0.8750 | 0.8184 | 0.6533 | 0.081* |
| C6 | 0.8898 (4) | 0.7412 (2) | 0.5694 (3) | 0.0661 (13) |
| H6 | 0.9074 | 0.7667 | 0.5206 | 0.079* |
| C7 | 0.8844 (3) | 0.6714 (2) | 0.5609 (3) | 0.0507 (10) |
| C8 | 0.8573 (3) | 0.63328 (19) | 0.6355 (3) | 0.0433 (9) |
| C9 | 0.8534 (3) | 0.5631 (2) | 0.6255 (3) | 0.0525 (11) |
| H9 | 0.8374 | 0.5371 | 0.6744 | 0.063* |
| C10 | 0.8724 (4) | 0.5324 (2) | 0.5464 (4) | 0.0665 (13) |
| H10 | 0.8690 | 0.4860 | 0.5416 | 0.080* |
| C11 | 0.8969 (4) | 0.5702 (3) | 0.4727 (4) | 0.0741 (14) |
| H11 | 0.9087 | 0.5489 | 0.4182 | 0.089* |
| C12 | 0.9039 (3) | 0.6382 (3) | 0.4795 (3) | 0.0666 (13) |
| H12 | 0.9216 | 0.6629 | 0.4301 | 0.080* |
| C13 | 0.4383 (3) | 0.44910 (18) | 0.5645 (2) | 0.0421 (9) |
| H13 | 0.3634 | 0.4697 | 0.5500 | 0.050* |
| C14 | 0.5879 (3) | 0.38798 (17) | 0.5476 (3) | 0.0428 (9) |
| C15 | 0.6185 (3) | 0.41847 (17) | 0.6388 (2) | 0.0370 (8) |
| C16 | 0.7297 (3) | 0.40796 (19) | 0.7041 (3) | 0.0515 (10) |
| H16 | 0.7507 | 0.4278 | 0.7653 | 0.062* |
| C17 | 0.8083 (4) | 0.3663 (2) | 0.6737 (4) | 0.0638 (12) |
| H17 | 0.8842 | 0.3582 | 0.7154 | 0.077* |
| C18 | 0.7766 (4) | 0.3365 (2) | 0.5830 (4) | 0.0684 (13) |
| H18 | 0.8319 | 0.3087 | 0.5658 | 0.082* |
| C19 | 0.6675 (4) | 0.34618 (19) | 0.5176 (3) | 0.0556 (11) |
| H19 | 0.6472 | 0.3261 | 0.4565 | 0.067* |
| N1 | 0.5211 (2) | 0.45750 (13) | 0.64759 (19) | 0.0380 (7) |
| N2 | 0.4725 (3) | 0.40802 (14) | 0.5028 (2) | 0.0434 (8) |
| H2 | 0.4300 | 0.3964 | 0.4458 | 0.052* |
| Ni1 | 0.5000 | 0.52246 (3) | 0.7500 | 0.0369 (2) |
| O2 | 0.6755 (2) | 0.54170 (12) | 0.82476 (17) | 0.0469 (7) |
| O4 | 0.6028 (2) | 0.60642 (12) | 0.69919 (17) | 0.0441 (6) |
| O1W | 0.5000 | 0.7341 (3) | 0.7500 | 0.163 (4) |
| H1A | 0.541 (8) | 0.711 (4) | 0.716 (8) | 0.245* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.038 (2) | 0.052 (2) | 0.032 (2) | −0.0045 (18) | 0.0159 (17) | −0.0054 (18) |
| C2 | 0.042 (2) | 0.069 (3) | 0.048 (2) | −0.011 (2) | 0.0140 (18) | 0.000 (2) |
| C3 | 0.028 (2) | 0.054 (3) | 0.056 (2) | −0.0035 (18) | 0.0110 (17) | 0.001 (2) |
| C4 | 0.047 (3) | 0.058 (3) | 0.073 (3) | −0.003 (2) | 0.019 (2) | −0.010 (2) |
| C5 | 0.057 (3) | 0.047 (3) | 0.097 (4) | −0.007 (2) | 0.017 (3) | 0.012 (3) |
| C6 | 0.052 (3) | 0.074 (4) | 0.074 (3) | −0.004 (2) | 0.019 (2) | 0.022 (3) |
| C7 | 0.032 (2) | 0.066 (3) | 0.054 (3) | 0.001 (2) | 0.0117 (18) | 0.007 (2) |
| C8 | 0.0237 (19) | 0.048 (3) | 0.057 (2) | 0.0011 (17) | 0.0101 (17) | 0.006 (2) |
| C9 | 0.034 (2) | 0.057 (3) | 0.068 (3) | −0.0009 (19) | 0.017 (2) | 0.000 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.042 (3) | 0.070 (3) | 0.086 (3) | 0.011 (2) | 0.015 (2) | −0.020 (3) |
| C11 | 0.044 (3) | 0.109 (4) | 0.069 (3) | 0.021 (3) | 0.014 (2) | −0.021 (3) |
| C12 | 0.041 (3) | 0.107 (4) | 0.055 (3) | 0.009 (3) | 0.018 (2) | 0.009 (3) |
| C13 | 0.041 (2) | 0.046 (2) | 0.042 (2) | −0.0002 (18) | 0.0162 (18) | 0.0009 (18) |
| C14 | 0.049 (2) | 0.040 (2) | 0.046 (2) | −0.0024 (19) | 0.0236 (19) | 0.0021 (18) |
| C15 | 0.036 (2) | 0.038 (2) | 0.040 (2) | −0.0002 (17) | 0.0171 (17) | 0.0012 (17) |
| C16 | 0.045 (2) | 0.052 (3) | 0.058 (3) | 0.003 (2) | 0.016 (2) | 0.002 (2) |
| C17 | 0.043 (3) | 0.060 (3) | 0.088 (3) | 0.008 (2) | 0.016 (2) | 0.004 (3) |
| C18 | 0.064 (3) | 0.060 (3) | 0.094 (4) | 0.015 (2) | 0.043 (3) | −0.004 (3) |
| C19 | 0.064 (3) | 0.052 (3) | 0.061 (3) | 0.000 (2) | 0.035 (2) | −0.006 (2) |
| N1 | 0.0346 (17) | 0.0430 (18) | 0.0379 (16) | 0.0012 (14) | 0.0127 (14) | 0.0027 (14) |
| N2 | 0.045 (2) | 0.0480 (19) | 0.0362 (16) | −0.0053 (16) | 0.0095 (15) | −0.0029 (15) |
| Ni1 | 0.0321 (4) | 0.0448 (4) | 0.0365 (4) | 0.000 | 0.0142 (3) | 0.000 |
| O2 | 0.0376 (15) | 0.0565 (17) | 0.0476 (15) | −0.0063 (12) | 0.0132 (12) | 0.0065 (13) |
| O4 | 0.0357 (15) | 0.0578 (17) | 0.0412 (14) | −0.0039 (12) | 0.0143 (12) | −0.0008 (12) |
| O1W | 0.097 (5) | 0.066 (4) | 0.320 (13) | 0.000 | 0.046 (6) | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—O2 | 1.254 (4) | C13—N1 | 1.316 (4) |
| C1—O4 | 1.260 (4) | C13—N2 | 1.341 (4) |
| C1—C2 | 1.516 (5) | C13—H13 | 0.9300 |
| C1—Ni1 | 2.498 (4) | C14—N2 | 1.374 (4) |
| C2—C3 | 1.502 (5) | C14—C15 | 1.394 (5) |
| C2—H2A | 0.9700 | C14—C19 | 1.395 (5) |
| C2—H2B | 0.9700 | C15—C16 | 1.383 (5) |
| C3—C4 | 1.361 (5) | C15—N1 | 1.405 (4) |
| C3—C8 | 1.429 (5) | C16—C17 | 1.389 (5) |
| C4—C5 | 1.403 (6) | C16—H16 | 0.9300 |
| C4—H4 | 0.9300 | C17—C18 | 1.382 (6) |
| C5—C6 | 1.356 (6) | C17—H17 | 0.9300 |
| C5—H5 | 0.9300 | C18—C19 | 1.364 (6) |
| C6—C7 | 1.401 (6) | C18—H18 | 0.9300 |
| C6—H6 | 0.9300 | C19—H19 | 0.9300 |
| C7—C12 | 1.410 (5) | N1—Ni1 | 2.021 (3) |
| C7—C8 | 1.413 (5) | N2—H2 | 0.8600 |
| C8—C9 | 1.410 (5) | Ni1—N1$^{i}$ | 2.021 (3) |
| C9—C10 | 1.355 (5) | Ni1—O2 | 2.055 (2) |
| C9—H9 | 0.9300 | Ni1—O2$^{i}$ | 2.055 (2) |
| C10—C11 | 1.386 (6) | Ni1—O4 | 2.287 (2) |
| C10—H10 | 0.9300 | Ni1—O4$^{i}$ | 2.288 (2) |
| C11—C12 | 1.364 (6) | Ni1—C1$^{i}$ | 2.498 (4) |
| C11—H11 | 0.9300 | O1W—H1A | 0.90 (8) |
| C12—H12 | 0.9300 | | |
| | | | |
| O2—C1—O4 | 120.7 (3) | C14—C15—N1 | 108.8 (3) |
| O2—C1—C2 | 118.1 (3) | C15—C16—C17 | 116.6 (4) |
| O4—C1—C2 | 121.2 (3) | C15—C16—H16 | 121.7 |
| O2—C1—Ni1 | 55.05 (17) | C17—C16—H16 | 121.7 |
| O4—C1—Ni1 | 65.66 (19) | C18—C17—C16 | 121.6 (4) |

| | | | |
|---|---|---|---|
| C2—C1—Ni1 | 172.8 (3) | C18—C17—H17 | 119.2 |
| C3—C2—C1 | 116.6 (3) | C16—C17—H17 | 119.2 |
| C3—C2—H2A | 108.1 | C19—C18—C17 | 122.7 (4) |
| C1—C2—H2A | 108.1 | C19—C18—H18 | 118.7 |
| C3—C2—H2B | 108.1 | C17—C18—H18 | 118.7 |
| C1—C2—H2B | 108.1 | C18—C19—C14 | 116.1 (4) |
| H2A—C2—H2B | 107.3 | C18—C19—H19 | 122.0 |
| C4—C3—C8 | 118.6 (4) | C14—C19—H19 | 122.0 |
| C4—C3—C2 | 120.9 (4) | C13—N1—C15 | 104.6 (3) |
| C8—C3—C2 | 120.5 (4) | C13—N1—Ni1 | 122.2 (2) |
| C3—C4—C5 | 121.7 (4) | C15—N1—Ni1 | 132.9 (2) |
| C3—C4—H4 | 119.2 | C13—N2—C14 | 107.3 (3) |
| C5—C4—H4 | 119.2 | C13—N2—H2 | 126.4 |
| C6—C5—C4 | 120.2 (4) | C14—N2—H2 | 126.4 |
| C6—C5—H5 | 119.9 | N1—Ni1—N1$^{i}$ | 100.03 (15) |
| C4—C5—H5 | 119.9 | N1—Ni1—O2 | 101.45 (10) |
| C5—C6—C7 | 120.8 (4) | N1$^{i}$—Ni1—O2 | 92.41 (10) |
| C5—C6—H6 | 119.6 | N1—Ni1—O2$^{i}$ | 92.41 (10) |
| C7—C6—H6 | 119.6 | N1$^{i}$—Ni1—O2$^{i}$ | 101.45 (10) |
| C6—C7—C12 | 121.8 (4) | O2—Ni1—O2$^{i}$ | 158.42 (14) |
| C6—C7—C8 | 119.1 (4) | N1—Ni1—O4 | 93.73 (10) |
| C12—C7—C8 | 119.1 (4) | N1$^{i}$—Ni1—O4 | 151.40 (10) |
| C9—C8—C7 | 117.9 (4) | O2—Ni1—O4 | 60.13 (9) |
| C9—C8—C3 | 122.4 (4) | O2$^{i}$—Ni1—O4 | 102.90 (9) |
| C7—C8—C3 | 119.6 (4) | N1—Ni1—O4$^{i}$ | 151.40 (10) |
| C10—C9—C8 | 121.7 (4) | N1$^{i}$—Ni1—O4$^{i}$ | 93.73 (10) |
| C10—C9—H9 | 119.1 | O2—Ni1—O4$^{i}$ | 102.90 (9) |
| C8—C9—H9 | 119.1 | O2$^{i}$—Ni1—O4$^{i}$ | 60.13 (9) |
| C9—C10—C11 | 120.1 (4) | O4—Ni1—O4$^{i}$ | 85.60 (12) |
| C9—C10—H10 | 120.0 | N1—Ni1—C1 | 99.19 (11) |
| C11—C10—H10 | 120.0 | N1$^{i}$—Ni1—C1 | 121.98 (11) |
| C12—C11—C10 | 120.6 (4) | O2—Ni1—C1 | 30.01 (10) |
| C12—C11—H11 | 119.7 | O2$^{i}$—Ni1—C1 | 131.69 (12) |
| C10—C11—H11 | 119.7 | O4—Ni1—C1 | 30.12 (10) |
| C11—C12—C7 | 120.6 (4) | O4$^{i}$—Ni1—C1 | 94.46 (11) |
| C11—C12—H12 | 119.7 | N1—Ni1—C1$^{i}$ | 121.98 (11) |
| C7—C12—H12 | 119.7 | N1$^{i}$—Ni1—C1$^{i}$ | 99.19 (11) |
| N1—C13—N2 | 113.5 (3) | O2—Ni1—C1$^{i}$ | 131.69 (12) |
| N1—C13—H13 | 123.3 | O2$^{i}$—Ni1—C1$^{i}$ | 30.01 (10) |
| N2—C13—H13 | 123.3 | O4—Ni1—C1$^{i}$ | 94.46 (11) |
| N2—C14—C15 | 105.9 (3) | O4$^{i}$—Ni1—C1$^{i}$ | 30.12 (10) |
| N2—C14—C19 | 132.2 (4) | C1—Ni1—C1$^{i}$ | 115.13 (18) |
| C15—C14—C19 | 122.0 (4) | C1—O2—Ni1 | 94.9 (2) |
| C16—C15—C14 | 121.1 (3) | C1—O4—Ni1 | 84.2 (2) |
| C16—C15—N1 | 130.1 (3) | | |

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|---|---|---|---|
| O2—C1—C2—C3 | 159.6 (3) | C13—N1—Ni1—O2 | −156.1 (3) |
| O4—C1—C2—C3 | −21.6 (5) | C15—N1—Ni1—O2 | 16.7 (3) |
| Ni1—C1—C2—C3 | 177 (2) | C13—N1—Ni1—O2$^{i}$ | 7.2 (3) |

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| C1—C2—C3—C4 | 113.3 (4) | C15—N1—Ni1—O2$^{i}$ | −180.0 (3) |
| C1—C2—C3—C8 | −66.9 (5) | C13—N1—Ni1—O4 | −95.9 (3) |
| C8—C3—C4—C5 | −0.9 (6) | C15—N1—Ni1—O4 | 76.9 (3) |
| C2—C3—C4—C5 | 178.9 (4) | C13—N1—Ni1—O4$^{i}$ | −8.2 (4) |
| C3—C4—C5—C6 | 1.7 (6) | C15—N1—Ni1—O4$^{i}$ | 164.6 (2) |
| C4—C5—C6—C7 | −1.2 (6) | C13—N1—Ni1—C1 | −125.7 (3) |
| C5—C6—C7—C12 | 179.4 (4) | C15—N1—Ni1—C1 | 47.1 (3) |
| C5—C6—C7—C8 | 0.1 (6) | C13—N1—Ni1—C1$^{i}$ | 1.8 (3) |
| C6—C7—C8—C9 | −179.5 (3) | C15—N1—Ni1—C1$^{i}$ | 174.6 (3) |
| C12—C7—C8—C9 | 1.2 (5) | O2—C1—Ni1—N1 | −97.0 (2) |
| C6—C7—C8—C3 | 0.6 (5) | O4—C1—Ni1—N1 | 81.5 (2) |
| C12—C7—C8—C3 | −178.7 (3) | C2—C1—Ni1—N1 | −116 (2) |
| C4—C3—C8—C9 | 179.9 (3) | O2—C1—Ni1—N1$^{i}$ | 11.0 (2) |
| C2—C3—C8—C9 | 0.1 (5) | O4—C1—Ni1—N1$^{i}$ | −170.49 (17) |
| C4—C3—C8—C7 | −0.2 (5) | C2—C1—Ni1—N1$^{i}$ | −8 (2) |
| C2—C3—C8—C7 | −180.0 (3) | O4—C1—Ni1—O2 | 178.5 (3) |
| C7—C8—C9—C10 | −1.3 (5) | C2—C1—Ni1—O2 | −19 (2) |
| C3—C8—C9—C10 | 178.6 (4) | O2—C1—Ni1—O2$^{i}$ | 161.39 (15) |
| C8—C9—C10—C11 | 0.2 (6) | O4—C1—Ni1—O2$^{i}$ | −20.1 (3) |
| C9—C10—C11—C12 | 0.9 (6) | C2—C1—Ni1—O2$^{i}$ | 142 (2) |
| C10—C11—C12—C7 | −1.0 (6) | O2—C1—Ni1—O4 | −178.5 (3) |
| C6—C7—C12—C11 | −179.4 (4) | C2—C1—Ni1—O4 | 162 (2) |
| C8—C7—C12—C11 | −0.1 (6) | O2—C1—Ni1—O4$^{i}$ | 108.2 (2) |
| N2—C14—C15—C16 | 179.0 (3) | O4—C1—Ni1—O4$^{i}$ | −73.3 (2) |
| C19—C14—C15—C16 | −0.5 (5) | C2—C1—Ni1—O4$^{i}$ | 89 (2) |
| N2—C14—C15—N1 | −0.7 (4) | O2—C1—Ni1—C1$^{i}$ | 131.1 (2) |
| C19—C14—C15—N1 | 179.7 (3) | O4—C1—Ni1—C1$^{i}$ | −50.43 (17) |
| C14—C15—C16—C17 | 0.5 (5) | C2—C1—Ni1—C1$^{i}$ | 112 (2) |
| N1—C15—C16—C17 | −179.8 (3) | O4—C1—O2—Ni1 | −1.6 (4) |
| C15—C16—C17—C18 | −0.4 (6) | C2—C1—O2—Ni1 | 177.3 (3) |
| C16—C17—C18—C19 | 0.4 (7) | N1—Ni1—O2—C1 | 88.6 (2) |
| C17—C18—C19—C14 | −0.4 (6) | N1$^{i}$—Ni1—O2—C1 | −170.7 (2) |
| N2—C14—C19—C18 | −179.0 (4) | O2$^{i}$—Ni1—O2—C1 | −40.39 (19) |
| C15—C14—C19—C18 | 0.5 (6) | O4—Ni1—O2—C1 | 0.86 (19) |
| N2—C13—N1—C15 | 0.3 (4) | O4$^{i}$—Ni1—O2—C1 | −76.3 (2) |
| N2—C13—N1—Ni1 | 174.9 (2) | C1$^{i}$—Ni1—O2—C1 | −66.1 (3) |
| C16—C15—N1—C13 | −179.5 (4) | O2—C1—O4—Ni1 | 1.4 (3) |
| C14—C15—N1—C13 | 0.3 (4) | C2—C1—O4—Ni1 | −177.4 (3) |
| C16—C15—N1—Ni1 | 6.8 (6) | N1—Ni1—O4—C1 | −101.9 (2) |
| C14—C15—N1—Ni1 | −173.4 (2) | N1$^{i}$—Ni1—O4—C1 | 17.0 (3) |
| N1—C13—N2—C14 | −0.8 (4) | O2—Ni1—O4—C1 | −0.86 (19) |
| C15—C14—N2—C13 | 0.9 (4) | O2$^{i}$—Ni1—O4—C1 | 164.7 (2) |
| C19—C14—N2—C13 | −179.5 (4) | O4$^{i}$—Ni1—O4—C1 | 106.7 (2) |
| C13—N1—Ni1—N1$^{i}$ | 109.3 (3) | C1$^{i}$—Ni1—O4—C1 | 135.57 (19) |
| C15—N1—Ni1—N1$^{i}$ | −77.9 (3) | | |

Symmetry code: (i) $-x+1, y, -z+3/2$.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*A*···O4 | 0.90 (8) | 2.24 (8) | 2.988 (6) | 141 (8) |
| N2—H2···O4$^{ii}$ | 0.86 | 2.00 | 2.791 (4) | 152 |

Symmetry code: (ii) −*x*+1, −*y*+1, −*z*+1.